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Pre and Post Processing for Large Scale Computations in Optimal Design and Control

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THE AIR FORCE CENTER FOR OPTIMAL DESIGN AND CONTROL

for the period

1 May 1997 - 30 April 1998

by

J. A. Burns and E. M. Cliff
Center for Optimal Design and Control

Wright House / West Campus Drive
Virginia Polytechnic Institute & State University
Blacksburg, VA 24061- 0531

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J.A. Burns

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Interdisciplinary Center for Applied Mathematics
Wright House, West Campus Drive
Virginia Polytechnic Institute and State University
Blacksburg, Virginia 24061-0531

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13. ABSTRACT *(Maximum 200 words)*

This report contains a summary and highlights of the work funded by the Air Force under AFOSR Grant F49620-97-1-0304, titled "Pre- and Post-processing for Large Scale Computations in Optimal Design & Control". This effort, funded under the Defense University Research Instrumentation Program (DURIP), was conducted by the Center for Optimal Design and Control (**CODAC**), at Virginia Tech during the period 1 May 1997 – 30 April 1998.

The objective of the grant was to provide enhanced computational and graphical facilities for a sensitivity-based design environment. In recent years researchers at **CODAC** have developed mathematical foundations and a computational framework for the rapid calculation of design-sensitivities for aerospace applications. Implementation requires approximate solution of certain linear partial differential equation. In aerodynamic applications, for example, these solutions describe in linear approximation how the flow will change with a given change in a (geometric) design parameter. We have acquired an SGI Onyx Workstation with four processors and a Fore Systems Asynchronous Transfer Mode (ATM) data switch with twelve ports which greatly enhance our abilities in graphical representations.

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Chapter 1

Introduction

This grant was awarded under the Defense University Research Instrumentation Program (DURIP) and has provided support for equipment to enhance the capabilities of the **PRET- CODAC** researchers to develop and utilize tools that will facilitate engineering design. We have acquired a powerful computational and graphics platform that is being used for development of interactive design tools, as well as in our work on scientific computation/visualization,

The Air Force Center for Optimal Design And Control (**CODAC**), established in 1993, addresses a number of technological thrusts related to these key components. **CODAC** researchers have made significant progress in these areas and our industrial partners: AeroSoft, BEAM Technologies, Boeing Defense and Space Group, give us a proven team of scientists and engineers from small high-tech firms and major aerospace companies. The research group at Virginia Tech has been at the forefront of the development of sensitivity methods for optimal design, with applications to shape optimization for fluid flow management. AeroSoft provides expertise in computational methods for optimization and for simulation of fluid dynamics.

CODAC is funded by the Air Force Office of Scientific Research through the Air Force Program for Research Excellence and Transition (*PRET*) under (Grant AFOSR–49620–96–1–0329). Dr. John A. Burns, Hatcher Professor of Mathematics at VPI & SU, is the Director of **CODAC** and principal investigator on the project. Dr. Marc Jacobs, AFOSR/NM is the technical monitor. **CODAC** is located within the Interdisciplinary Center for Applied Mathematics (**ICAM**) at Virginia Tech. Dr. Terry L. Herdman, Professor of Mathematics at VPI & SU,is the Director of **ICAM**.

Chapter 2

Status and Highlights

2.1 Equipment Purchased

The principal equipment purchased under the grant were:

1. an Onyx Reality Engine Deskside System from Silicon Graphics Inc., featuring
   - (4) R10000, 195 MHz CPU's, with 512 MB RAM memory,
   - a Sirius Video digital video system,
   - a 21" Super-Wide color monitor; and,
2. a Workgroup ATM Switch from Fore Systems Inc. including:
   - twelve ATM ports,
   - five ATM boards for SGI and DEC platforms.

This equipment has been integrated into the **ICAM** computer network.

2.2 Current Computing Facilities

ICAM houses a heterogeneous Unix system with file-sharing under a Network File System (NFS). The Unix system currently consists of the following components:

- Our main file server is four processor SUN-1000, with 128MB internal memory. An external cabinet houses approximately 100GB of disk space through a SCSI connection.
- Our graphics workstations include a Silicon Graphics Onyx2 with Infinite Reality graphics and four R10000 processors, four single-processor (R10000) Octane workstations, and an SGI IRIS 4D/310 graphics workstations. Two SGI-Indigo2 workstations feature R8000 processors, 128MB of memory and Extreme graphics.
- Our main computational platform is a SGI Origin 2000 with 16 R10000 processors and 18GB of memory (`origin.icam.vt.edu`). This machine, which operates in the range of 10 GF, supports interactive use and batch use under the Network Queuing System (NQS). The machine can be dedicated to a single-user for particularly challenging computations.
- Additionally, we support two DEC Alpha 3000/600 computers with 256MB of memory. A third DEC AlphaServer 2100 is a dual-processor machine with 512MB of memory.
- The system is connected via an Asynchronous Transfer Mode network (ATM - OC3, 155 Mb/s) and by switched-Ethernet.

Chapter 3

Accomplishments

The equipment purchased under this grant has enhanced our abilities to do fundamental research and has opened new possibilities for the industrial transition of our work. In this report we focus on the this latter aspect.

3.1 Development of Interactive Design Tools

In recent years there has been a great deal of research into use of optimization-based algorithms in aerodynamic design (see [5, 6]). This emphasis has spurred the need for design sensitivities and for efficient ways to calculate them. At this point the approaches available for the calculation of design sensitivities may be sorted into four categories:

1. finite difference of neighboring solutions
2. 'differentiate' the numerical code (*i.e.* ADIFOR)
3. 'adjoint' methods
4. 'differentiate' the boundary-value problem

The first approach is costly and while apparently straight-forward, there are inevitable difficulties with choices of step-size and the interaction with solution accuracy [8]. The second approach formally applies the chain-rule to each line of code to produce another code which will evaluate the derivatives [2, 3, 7]. This again, seems straightforward but there are important issues when one wishes to retain computational efficiency of the original CFD solver. The third approach [11, 12, 13], relies on functional analysis and can be difficult to justify rigorously.

Our research group has focused on the fourth approach, often called the Sensitivity Equation Method (SEM) [1, 4, 9], A high-level view of the abstract SEM approach is that it produces a *linear* boundary-value problem; the solution of this problem is a flow sensitivity and describes, in linear approximation, the way the flow solution (dependent variables) depends on a (scalar) design parameter. In applications one finds that the solution of the underlying nonlinear boundary-value problem often relies on a linearization so that many of the required ingredients for the SEM already exist within a basic CFD code. This is the idea implemented in the *SENSE* code from AeroSoft Inc [10], one of our PRET industrial partners.

3.2 Sensitivity Analysis

The sensitivity implementation in *SENSE* is fundamentally based on implicit-differentiation applied to the boundary-value problem describing the fluid mechanics. That is, one envisions an implicit

equation

$$\mathcal{R}(\mathbf{Q}, \beta) = 0, \tag{3.1}$$

where $\mathbf{Q}$ denotes the distributed dependent variables (*e.g.* density, momentum, energy) and β denotes a design variable. For fixed β the equation (3.1) is solved for $\mathbf{Q}$. This defines a map

$$\beta \rightarrow \mathbf{Q},$$

which associates a flow solution with the specified design parameter(s). The sensitivity is the derivative of this map; it provides a linear approximation for how the flow solution will change under a small change in the design parameter. One proceeds by formally differentiating (3.1) to produce

$$\frac{\partial \mathcal{R}}{\partial u}\frac{\partial u}{\partial \beta} + \frac{\partial \mathcal{R}}{\partial \beta} = 0. \tag{3.2}$$

The *SENSE* code implements a numerical approximation to (3.2) for situations wherein $\mathcal{R}$ models Reynolds-Averaged Navier-Stokes flows with finite-rate chemistry.

The integral equations for the fluid dynamic system are written as

$$\frac{\partial}{\partial t}\iiint \mathbf{Q}\, dV + \oint_A (\mathbf{F}(\mathbf{Q}) \cdot \hat{\mathbf{n}})\, dA = \oint_A (\mathbf{F}_v(\mathbf{Q}) \cdot \hat{\mathbf{n}})\, dA + \iiint \mathbf{S}\, dV, \tag{3.3}$$

where $\mathbf{Q} = \mathbf{Q}(x, y, z, t; \beta)$ represents the vector of state variables resulting from conservation of mass, momentum and energy. The surface integrals represent the inviscid and viscous fluxes ($\mathbf{F}$ and $\mathbf{F}_v$). Changes in chemical composition are governed by the species production terms in the source term $\mathbf{S}$. Formal differentiation of the integral equation in equation (3.3) with respect to a generic design variable (denoted as β) results in the sensitivity equations. These equations are linear in the sensitivities. Presented in integral form, they are

$$\frac{\partial}{\partial t}\iiint \mathbf{Q}'\, dV + \oint_A (\mathbf{F}'(\mathbf{Q}) \cdot \hat{\mathbf{n}})\, dA = \oint_A (\mathbf{F}'_v(\mathbf{Q}) \cdot \hat{\mathbf{n}})\, dA + \iiint \mathbf{S}'\, dV, \tag{3.4}$$

where $\mathbf{Q}'$ is the flow sensitivity, $\partial(\mathbf{Q})/\partial\beta$. *SENSE* solves equation (3.4) using an upwind characteristic-based formulation.

3.3 Design Environments

The result of solving the *continuous sensitivity* equation (3.4) is a collection of field functions describing, for example, the sensitivity of density, momenta and energy to changes in a parameter of interest. We have explored some ideas for using graphical workstations to present such information to the designer.

Shown in Figure 1 is a screen image for one such implementation. In the upper left we display the basic pressure distribution in the two-dimensional flow-field. The sub-figure in the upper-right displays the sensitivity of the pressure to a change in the design variable (here the angle of attack) from its nominal value. Also visible on the right-side of the screen is a collection of menus including a *slider* that enables one to specify an increment in the design-variable. Finally, the large image at the bottom displays the *Taylor series approximation*, that is, the basic flow plus the product of the sensitivity and the design-increment. By moving the slider the designer sees instantly an estimate of how the pressure field will change under a change in the design variable. Other menus in the window allow the designer to select different field-variables for display (e.g. the density) or change the countour display. We are pursuing other ideas for using sensitivities to provide additional insight to a human designer. The graphical and computational capabilities of the *Onyx* workstation are crucial for these implementations.

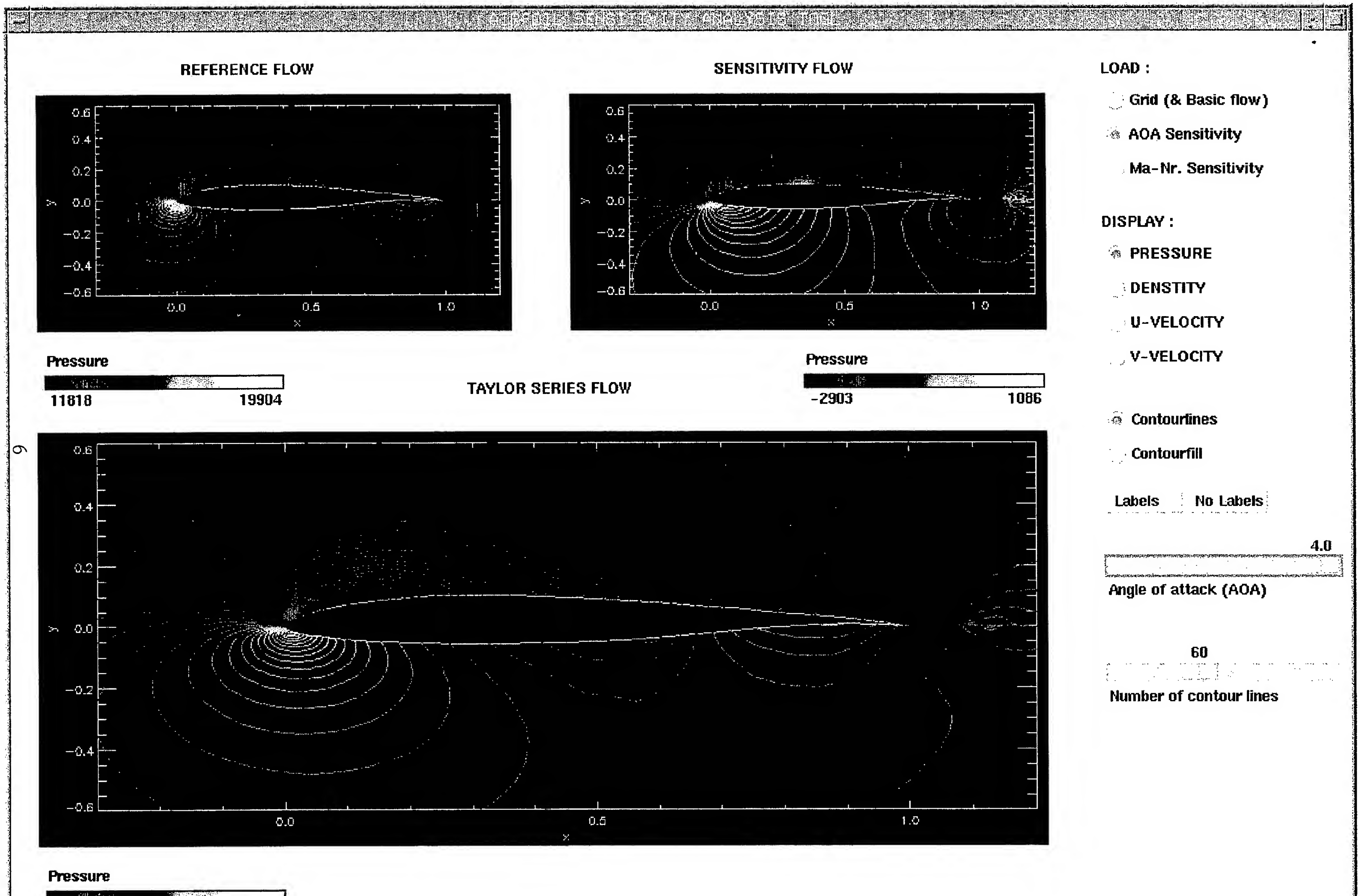

Figure 1: Screen Image of a Design Environment

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